KFM 11: Focus Session: (Multi-)Ferroic States II

The focus session is dedicated to (multi)ferroic states at interfaces and in heterostructures. The design of (emergent) properties at interfaces, modelling methods and advanced characterization tools will be of interest. Typical examples may include electrostatic and strain boundary conditions at interfaces, domains and domain walls in (multi)ferroics and applications in nano-electronic device

Chair: Nives Strkalj (Institute of Physics, Zagreb)

Time: Tuesday 9:30–12:20 Location: EMH 225

KFM 11.1 Tue 9:30 EMH 225

Polar textures on silicon — •Catherine Dubourdieu — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — Freie Universität Berlin, Berlin, Germany

In nanoscale ferroelectrics, the polarization pattern depends on the chemical, mechanical and electrical boundary conditions and is the result of a delicate balance to minimize electrostatic energy costs associated with the depolarization field. In recent years, new exotic polar textures featuring curled polarization patterns (vortices, skyrmions, merons, etc...) have been unraveled in ultrathin films, superlattices or nanostructures. The development of topological nanoelectronics on chips that would take advantage of such polar nanodomains requires their integration on silicon. I will present in this talk the growth and the resulting polarization patterns of (BaTiO3/SrTiO3)n superlattices and of BaTiO3 nanoislands on silicon substrates. The epitaxy on Si of both types of heterostructures is realized by molecular beam epitaxy, which will be detailed. Based on X-ray diffraction, scanning transmission electron microscopy and piezoresponse force microscopy characterizations, I will discuss the strain state, the peculiar polar textures that develop in these systems and their response under electric field. The evidence of curled polarization nanodomains in the different BaTiO3-based heterostructures is a first step towards the integration of topological defects into nanoscale devices.

KFM 11.2 Tue 10:00 EMH 225

In-situ monitoring of polarization dynamics during the epitaxial integration of $BaTiO_3$ thin films on silicon templates — •Bixin Yan, Ipek Efe, Manfred Fiebig, and Morgan Trassin — Department of Materials, ETH Zurich, Switzerland

Ferroelectric oxides host technologically-relevant properties, and their integration onto the CMOS-compatible silicon platform is key for the next generation of oxide electronics. However, the interplay of thermal coefficient mismatch and strain relaxation during the growth of ferroelectric epitaxial thin films on silicon results in a multi-domain configuration in the films, deviating from the application-relevant single-domain state. Here, taking $BaTiO_3$ as our ferroelectric model system, we directly investigate the polarization state of our films during the pulsed laser deposition growth on $SrTiO_3$ (STO)-buffered silicon using in-situ optical second harmonic generation (ISHG). We monitor the emergence of out-of-plane polarization in the early stage of the growth and track in real-time the thickness-dependent in-plane polarized domain formation induced by interfacial strain relaxation. We shed light on the role of growth conditions on the final polarization state of our films and compare the observed behavior with the case of coherently strained thin films grown on conventional single crystalline STO substrates. Finally, ISHG measurements during post-growth cooldown isolate the impact of thermal expansion coefficient mismatch in the final domain architecture in the films. Hence, our work provides new insights into the integration of ferroelectric oxides on silicon templates, a necessary step for the realization of energy-efficient technologies.

KFM 11.3 Tue 10:20 EMH 225

Epitaxial Strain in Arbitrary Orientation in BaTiO3 films and BaTiO3/SrTiO3 superlattices — •Lan-Tien Hsu[1], Anna Grünebohm[1], and Frank Wendler[2] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany — [2]Institute of Materials Simulation, Department of Materials Science, Friedrich-Alexander University of Erlangen-Nürnberg, Dr.-Mack-Strasse 77, 90762 Fürth, Germany

Interface strain plays a crucial role in ferroelectric thin films and multilayer systems, which have potential in e.g. high-frequency capacitors and random-access memories[1]. Epitaxial (001), (110), and (111) strains can alter phase stability and enhance ferroelectric properties in BaTiO3 films[2]. However, it is still unclear how the epitaxial strain in low symmetric orientation influences films and multilayer systems.

In this work, we study the epitaxial strain in low symmetric orientations in bulk-like BaTiO3 (without a depolarization field) and in BaTiO3/SrTiO3 superlattices, using ab initio based coarse-grained molecular dynamics[3]. Complex multidomain structures appear, particularly in superlattices due to the presence of depolarization fields. Furthermore, we compare these strain-induced phases with those induced by electric fields along arbitrary directions.

[1] A. Grünebohm et al., J. Phys. 34, 2021
[2] H. Wu et al., AIP Advances 6, 2016
[3] T. Nishimatsu et al., Phys. Rev. B 78, 2008

KFM 11.4 Tue 10:40 EMH 225

Interplay of layer and spontaneous polarization in superlattices of metallic $SmNiO_3$ and ferroelectric $BaTiO_3$ — •Edith Simmen and Nicola A. Spaldin — Materials Theory, ETH Zurich, Switzerland

We present a density functional theory (DFT) study of superlattices containing metallic $SmNiO_3$ (SNO) and ferroelectric $BaTiO_3$ (BTO). The interface of SNO with BTO hosts numerous interesting functionalities which can compete or cooperate: Since BTO and SNO are II-IV and III-III perovskites, respectively, the different layer charges lead to a built-in polar discontinuity in addition to the spontaneous polarization of BTO. These two sources of polarization can both interact with each other and with the SNO via its metallic screening. We find that despite the metallicity of SNO, the polar electrostatics strongly affect the ground state. The system avoids a polar discontinuity by aligning the spontaneous polarization of the BTO parallel to the layer polarization of the SNO in the so-called 'happy' orientation. We find that this happy polarization is stable down to a single unit cell of BTO, in contrast to the 6-unit-cell critical thickness previously found for BTO with II-IV metallic electrodes [1]. The opposite 'unhappy' polarization orientation is however highly unfavoured, with the stability depending strongly on the thickness of the BTO layer and the tilts within the SNO layer.

[1] J. Junquera et al., Nature 422, 506 (2003)

10 min. break

Invited Talk KFM 11.5 Tue 11:10 EMH 225

Optical Formation and Manipulation of Topological Polar Supertextures — •John Freeland — X-ray Science Division, Argonne National Laboratory, Lemont, IL USA

Ultrafast stimuli can stabilize and control metastable states of matter inaccessible by equilibrium means. Establishing the spatiotemporal link between ultrafast excitation and metastability is crucial to understanding these phenomena. This talk will focus on superlattices of PbTiO3 (PTO) and SrTiO3 (STO) that host a variety of extended polar textures such as supercrystals, vortices, skyrmions, collectively dubbed polar supertextures. In particular we will explore the formation of polar supercrystals[1], which is a highly order phase created via optical excitation of these PTO/STO heterostructures. Since the transition is irreversible, an understanding of the formation pathway, we needed to use the high intensity ultrafast X-ray pulses from a free electron laser to track the single-shot dynamics of polar supercrystal creation from ps to us timescales. Together with dynamical phase field modeling, these results enabled tracking of the irreversible formation of this metastable polar supertexture and understanding of the creation process.

The work at Argonne is supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357. The development of the materials and ultrafast experiments is supported by the U.S. Department of Energy, Office of Science, Office of Basic

Energy Sciences under Award Number DE-SC-0012375.

[1] Stoica, V. A. et al. Nat. Mater. 18, 377 (2019).

KFM 11.6 Tue 11:40 EMH 225

Investigation of local structure in polar skyrmions using three-dimensional diffuse X-ray scattering — •Joohee Bang[1], Nives Strkalj[2], Martin Sarott[1], Morgan Trassin[1], and Thomas Weber[1] — [1]Department of Materials Science, ETH Zurich — [2]Institute of Physics, Zagreb

The discovery of nontrivial polar topologies have attracted great attention as it holds promise for alternative device configurations for microelectronics. Specifically, superlattices consisting of ferroelectric lead titanate and dielectric strontium titanate have shown a number of nontrivial topologies such as polar vortex-antivortex pairs [1] and polar skyrmions [2]. In fact, short-period (of only a few unit cells) superlattices were previously reported to exhibit improper ferroelectricity associated with octahedral tilts [3]. However, the phase and magnitude of octahedral tilts in the system are yet to be fully investigated. Detailed investigation of the local atomic structure and the interlayer correlation of the polarization domains in these nontrivial topological systems also remains elusive. Here, we perform an in-depth analysis of octahedral tilts as well as that of cation displacements in polar skyrmion structures via a comprehensive reciprocal space investigation. The observation of A-cation displacements associated with octahedral tilts as a function of temperature and the investigation of their correlation strength is the primary focus of our work.

[1]Yadav et al., Nature 530, 2016
[2]Das et al., Nature 568, 2019
[3]Bousquet et al., Nature 452, 2008

KFM 11.7 Tue 12:00 EMH 225

Brownian Electric Bubbles — •Hugo Aramberri[1] and Jorge Íñiguez-González[1,2] — [1]Luxembourg Institute of Science and Technology (LIST), Esch/Alzette, Luxembourg — [2]University of Luxembourg, Belvaux, Luxembourg

Magnetic skyrmions are point-like topological defects with a magnetization opposite to its embedding matrix. They have been studied for over a decade. Some of their most promising applications are in the field of unconventional computing, in which the stochastic motion of these nanometric objects plays a pivotal role. At the same time, electric skyrmion bubbles were recently predicted (and soon after experimentally confirmed) in electrostatically frustrated ferroelectrics. However, the field of electric bubbles is still at a nascent stage, and a fundamental characterization of these objects is still lacking. Importantly, the dynamics of electric bubbles still remain largely unexplored.

In this talk I will present second-principles atomistic molecular dynamics simulations of electric bubbles in ferroelectric/paraelectric superlattices ($PbTiO_3$/$SrTiO_3$), showing that they can present Brownian motion at room temperature. This work establishes the quasiparticle nature of electric bubbles, and sets the stage for their use as purely electric alternatives to magnetic skyrmions.

Aramberri and Íñiguez, arXiv:2308.01716 (2023).